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PRODGROUP - A PROGRAM FOR THE PRODUCTION OF MULTIGROUP REACTOR CONSTANTS FROM THE EVALUATED NUCLEAR DATA AVAILABLE AT IAEA

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PRODGROUP - A PROGRAM FOR THE PRODUCTION OF MULTIGROUP REACTOR CONSTANTS FROM THE EVALUATED NUCLEAR DATA AVAILABLE AT IAEA

by

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Abstract

The evaluated nuclear data files available at IAEA are used for generating multigroup constant sets for P_1 equations. The method of data handling and calculation is described and the corresponding computer program is presented.

Резюме

Масса оцененных ядерных данных, полученных от МАГАТЭ используются для произведения многогрупповых констант уравнений P_I. Описывается метод обработки данных и вычисления, а также соответствующая программа для ЭВМ.

Kivonat

Az IAEA-nál rendelkezésre álló kiértékelt nukleáris adatokat felhasználjuk a P_1 egyenletek sokcsoport-állandóinak előállitására. Ismertetjük a használt adatfeldolgozási és számitási módszereket, valamint a megfelelő számitógépi programot.

1. Introduction

The recent development of reactor calculations in our country [1] has required a reliable set of group constants. In the published literature there can be found some sets of microgroup constants, as, e.g. [2], [3], etc. These constants have been produced from evaluated nuclear data which originally resulted from nuclear theory and experiments. The group constants sets have been published over a relatively long period of time and they are not flexible enough as far as the calculation methods and special cicumstances are concerned, e.g. diffusion, transport and Monte Carlo calculation, heterogeneous systems, shielding calculations, etc.

Recently, evaluated data of some isotopes which are important in reactor physics have become available at IAEA on magnetic tape file. Therefore, to avoid the difficulties with the readymade group constants, a program has been prepared for their calculation from these evaluated data. It is hoped that in the future the accuracy of the nuclear data and the assortment of material available at IAEA will grow, thereby satisfying requirements concerned with the group constants in reactor physics calculations.

In this report a method for generating group constants for P_1 equations from evaluated data is outlined and the description of the related computer program is given.

2. Method for the calculation of group constants

The group constants are dependent on the equations in which they are to be used. For instance, a set of group constants prepared for S_n calculation is of doubtful applicability in diffusion calculation, and vice versa. Of course, if the energy mesh is small, i.e. the number of groups is large, then any set can be used for any purpose to a relatively good approximation. In the following only the calculation of group constants for P_1 approximation is considered; however, group constants for any other purposes could be obtained by similar consideration.

The P_1 equations in their general energy dependent form are:

$$\nabla J(r,E)+\Sigma(E)\phi(r,E) = \int dE'\Sigma_o(E'\to E)\phi(r,E') +\chi(E) \int dE'\ \nu(E')\Sigma_f(E')\phi(r,E') \qquad /2.1a/$$

$$1/3\ \nabla\phi(r,E) + \Sigma(E)\ J(r,E) = \int dE'\ \Sigma_1(E'\to E)\ J(r,E') \qquad /2.1b/$$

Multigroup equations can be obtained on the assumption that there is space-energy separability in the i-th group as

$$\phi(r,E) = \bar{\psi}(r)\ f(E) \qquad /2.2a/$$

$$J(r,E) = \bar{I}_i(r)\ j(E) \qquad /2.2b/$$

Inserting /2.2/ into the Eqs./2.1/ and integrating for E over the interval (E_{i+1}, E_i), we have

$$\nabla I_i(r) + \Sigma_o^i\ \psi_i(r) = \sum_{k\neq i} \Sigma_o^{k\to i}\ \psi_k(r) + \chi_i \sum_k (\nu\Sigma_f)^k\ \psi_k(r) \qquad /2.3a/$$

$$1/3\nabla\psi_i(r) + \Sigma_1^i\ I_i(r) = \sum_{k\neq i} \Sigma_1^{k\to i}\ I_k(r) \qquad /2.3b/$$

$$\Sigma_o^{k\to i} = \frac{\int_{E_{i+1}}^{E_i} dE \int_{E_{k+1}}^{E_k} dE'\ \Sigma_o(E'\to E)\ f(E')}{\int_{E_{k+1}}^{E_k} dE\ f(E)} \qquad /2.4a/$$

$$\Sigma_l^{k\to i} = \frac{\int_{E_{i+1}}^{E_i} dE \int_{E_{k+1}}^{E_k} dE'\ \Sigma_l(E'\to E)\, j(E')}{\int_{E_{k+1}}^{E_k} dE\ j(E)} \qquad /2.4b/$$

$$(\nu\Sigma_f)^i = \frac{\int_{E_{i+1}}^{E_i} dE'\ \nu(E')\ \Sigma_f(E')\ f(E')}{\int_{E_{i+1}}^{E_i} dE\ f(E)} \qquad /2.4c/$$

$$\chi_i = \int_{E_{i+1}}^{E_i} dE\ \chi(E) \qquad /2.4d/$$

$$\Sigma_o^i = \Sigma_{tf}^i - \Sigma_o^{i\to i} \qquad /2.4e/$$

$$\Sigma_l^i = \Sigma_{tj}^i - \Sigma_l^{i\to i} \qquad /2.4f/$$

$$\Sigma_{\substack{tf\\tj}}^i = \frac{\int_{E_{i+1}}^{E_i} dE\ \Sigma_t(E)\ \dfrac{f(E)}{j(E)}}{\int_{E_{i+1}}^{E'} dE\ \dfrac{f(E)}{j(E)}} \qquad /2.4g/$$

$$\psi_i(r) = \bar{\psi}(r) \int_{E_{i+1}}^{E_i} dE\ f(E).$$

$$I_i(r) = \bar{I}_i(r) \int_{E_{i+1}}^{E_i} dE\, j(E)$$

Over the thermal region, where there is no up-scattering, the equations become simpler. Namely, we may write $\sum_{k=1}^{i-1}$ instead of $\sum_{k\neq 1}$, and

$$\Sigma_{o\,1}^{i\to i} = \frac{\int_{E_{i+1}}^{E_i} dE \int_{E_{i+1}}^{E} dE'\, \Sigma_{o\,1}(E' \to E)\, j(E')\, f(E')}{\int_{E_{i+1}}^{E_i} dE\, j(E)\, f(E)}$$

In order to apply the above formulas, the energy spectra of flux and current, $f(E)$ and $j(E)$, should be known for every group. It is accepted that in the slowing-down region

$$f(E) = \frac{1}{E\Sigma(E)} \qquad /2.5a/$$

while in the thermal region

$$f(E) = \frac{E}{T^2}\, e^{-E/T} \qquad /2.5a'/$$

where T is the material temperature.

The discussion here will be confined to the energy range above the thermal region. Group constants in this region will be calculated in accordance with other types of considerations, making use of the results of the theory of inelastic scattering in solid or liquid phase.

Between $f(E)$ and $j(E)$ there is an approximate relation

$$j(E) = \frac{f(E)}{3\Sigma_{tr}(E)} \qquad /2.5b/$$

where $\Sigma_{tr}(E)$ is the transport cross-section.

In the higher energy region there would be a better but more complicated option than /2.5a/, as

$$f(E) = \frac{\int_{E}^{E_{max}} dE\ \psi(E)}{\Sigma(E)\ \Sigma E} + \chi(E) \qquad /2.5c/$$

/χ (E) is the fission spectrum./

Generally, in the slowing-down region three types of nuclear processes lead to the energy degradation of neutrons: elastic /Σ_{el}/ and inelastic /Σ_{in}/ scattering and the /n,2n/ process /$\Sigma_{n,2n}$/. Thus

$$\Sigma_o(E' \to E) = \Sigma_{el_o}(E' \to E) + \Sigma_{in}(E' \to E) + 2\Sigma_{n,2n}(E' \to E) \qquad /2.6a/$$

$$\Sigma_1(E' \to E) = \Sigma_{el_1}(E' \to E) \qquad /2.6b/$$

It is assumed that the inelastic scattering and the /n,2n/ process are isotropic in the laboratory system.

a/ Elastic scattering. Let $\sigma_s^{\ell}(E,\mu)$ be the differential elastic scattering cross-section in center-of-mass system, μ the cosine of scattering angle, M_ℓ the mass of the nucleus, and Q_ℓ the nuclear density, then /see [4]/

$$\int du'\ \Sigma_{el_o}(u' \to u)\ f(u') = \sum_{\ell} Q_\ell\ \frac{(M_\ell+1)^2}{4M_\ell} \int_{u-Q_\ell}^{u} du'\ f(u')\ \sigma_s^{\ell}\left(u', \mu(u,u')\right)\ e^{u'-u} \qquad /2.7a/$$

$$\int du'\ \Sigma_{el_1}(u' \to u)\ j(u') = \sum_{\ell} Q_\ell\ \frac{(M_\ell+1)^2}{4M_\ell} \int_{u-Q_\ell}^{u} du'\ j(u')\ \sigma_s^{\ell}\left(u', \mu(u,u')\right)\ e^{u'-u}$$

$$\left[\frac{M_\ell+1}{2}\, e^{-\frac{u-u'}{2}} - \frac{M_\ell-1}{2}\, e^{\frac{u-u'}{2}} \right] \qquad /2.7b/$$

where

$$q_\ell = \ln \frac{(M_\ell+1)^2}{(M_\ell-1)^2}$$

and

$$\mu(u,u') = 1 - \frac{(M_\ell+1)^2}{2M_\ell}\left(1 - e^{u'-u}\right) \qquad /2.8/$$

In these the more convenient lethargy variable is used instead of energy variable, i.e.

$$u = \ln E_o/E$$

Substituting /2.7/ into /2.4a-b/, we get

$$\Sigma_{el_o}^{k\to i} = \sum_\ell Q_\ell \frac{(M_\ell+1)^2}{4M_\ell} \varepsilon_{ki}^\ell \int_y^{u_{k+1}} du'\, f(u') \int_{w(u')}^{z(u)} \frac{du\, \sigma_s^\ell\left(u', \mu(u,u')\right) e^{u'-u}}{\int_{u_k}^{u_{k+1}} du\, f(u)}$$

$$\Sigma_{el_1}^{k\to i} = \sum_\ell Q_\ell \frac{(M_\ell+1)^2}{4M_\ell} \varepsilon_{ki}^\ell \int_y^{u_{k+1}} du'\, j(u') \int_{w(u')}^{z(u')} du\, \sigma_s^\ell\left(u', \mu(u,u')\right) e^{u'-u}$$

$$\left[\frac{M_\ell+1}{2} e^{-\frac{u-u'}{2}} - \frac{M_\ell-1}{2} e^{\frac{u-u'}{2}}\right] \Bigg/ \int_{u_k}^{u_{k+1}} du\, j(u) \qquad /2.9b/$$

$$\varepsilon_{ki} = \begin{cases} 1 & \text{if} \quad u_i - u_{k+1} \leq q \\ 0 & \text{if} \quad u_i - u_{k+1} > q \end{cases} \qquad /2.10a/$$

$$y = \begin{cases} u_k & \text{if} \quad u_i - u_k < q \\ u_i - q & \text{if} \quad u_i - u_k > q \end{cases} \qquad /2.10b/$$

$$z(u) = \begin{cases} u_{i+1} & u_{i+1} \leq q_\ell \\ u'+q_\ell & \text{otherwise} \end{cases} \qquad /2.10c/$$

$$w(u') = \begin{cases} u_i & \text{if} \quad i \neq k \\ u' & \text{if} \quad i = k \end{cases} \qquad /2.10d/$$

If the integral variable u is changed to μ in /2.9/, then we have

$$\Sigma_{el_o}^{k\to i} = \sum_\ell Q_\ell \frac{1}{2} \varepsilon_{ki}^\ell \int_y^{u_{k+1}} du' f(u') \int_{\mu(z,u')}^{\mu(w,u')} d\mu \, \sigma_s^\ell(u',\mu) \Big/ \int_{u_k}^{u_{k+1}} du f(u) \qquad /2.11a/$$

$$\Sigma_{el_1}^{k\to i} = \sum_\ell Q_\ell \frac{1}{2} \varepsilon_{ki}^\ell \int_y^{u_{k+1}} du' f(u') \int_{\mu(z,u')}^{\mu(w,u')} d\mu \, \sigma_s^\ell(u',\mu) \left[\frac{M_\ell+1}{2} \sqrt{1 - (1-\mu)\frac{2M_\ell}{(M_\ell+1)^2}} \right.$$

$$\left. - \frac{M_\ell-1}{2} \left(\sqrt{1 - (1-\mu)\frac{2M_\ell}{(M_\ell+1)^2}} \right)^{-1} \right] \Big/ \int_{u_k}^{u_{k+1}} du \, j(u) \qquad /2.11b/$$

If the scattering is isotropic in the center-of-mass system, i.e. $\sigma_s^\ell(u',\mu) = \sigma_s^\ell(u')$, then the inner integral in /2.11/ can be performed analytically, and we have

$$\Sigma_{el_o}^{k\to i} = \sum_\ell Q_\ell \frac{(M_\ell+1)^2}{4M_\ell} \varepsilon_{ki}^\ell \int_y^{u_{k+1}} du' f(u') \sigma_s^\ell \frac{(u') \, e^{u'} \left(e^{-u_i} - e^{-z(u')} \right)}{\int_{u_k}^{u_{k+1}} du f(u)} \qquad /2.12a/$$

$$\Sigma_{el}^{k\,i} = \sum_{\ell} Q_\ell \frac{(M_\ell+1)^2}{4M_\ell} \varepsilon_{ki}^{\ell} \int_{y}^{u_{k+1}} du'\, f(u')\, \sigma_s^{\ell}(u') \left[\frac{M_\ell+1}{3} e^{3/2u'} \left(e^{-3/2} - e^{w(u')-3/2(u')} \right) \right.$$

$$\left. - (M_\ell-1)\, e^{-u'/2} \left(e^{-w(u')/2} - e^{-\frac{z(u')}{2}} \right) \right] \qquad /2.12b/$$

b/ Inelastic scattering. Inelastic scattering of neutrons is treated in one of two ways, depending upon the energy of the incident neutron, E'. Let E_c denote a target nucleus excitation energy below which the level structure of the nucleus is given. In the process of inelastic scattering, the incident neutron loses an amount of energy approximately equal to the energy of excitation of the residual nucleus, E_i, i.e. more precisely

$$\sigma_{in}^{\ell}(E' \to E) = \sum_{i=1}^{c_\ell} \sigma_i^{\ell}(E')\, \delta\left(E - \frac{M_\ell-1}{M_\ell+1} E' + \frac{M_\ell}{M_\ell+1} E_i \right) \qquad /2.13/$$

/The sum is extended over the resolved excitation levels./

For $E' > E_c$ a continuous distribution, the so-called evaporation model, is used [5]:

$$\sigma_{in_{cont}}^{\ell}(E' \to E) = \sigma_{cont}^{\ell}(E') \frac{E\, e^{-E/\theta^{\ell}(E')}}{\theta^{\ell}(E') \left[\theta^{\ell}(E') - e^{-E'/\theta^{\ell}(E)} \left(\theta^{\ell}(E') + E' \right) \right]} \qquad /2.14/$$

where

$$\theta^{\ell}(E') = \sqrt{\frac{E'}{M_\ell}} \Big/ 0.31$$

Substituting /2.13/ and /2.14/ into /2.4a-b/, we obtain

$$\Sigma_{in}^{k\,j} = \sum_{\ell} Q_\ell \left[\sum_{i=1}^{c_\ell} \int_{E_{k+1}}^{E_k} dE'\, f(E')\, \sigma_i(E')\, \varepsilon_{kj}^{i} + \right.$$

$$\int_{E_{k+1}}^{E_k} dE'\ f(E')\ \sigma^{\ell}_{cont}(E)\ \frac{e^{-E_{j+1}/\Theta^{\ell}(E')}\left(\Theta^{\ell}(E')+E_{j+1}\right)-e^{-E_j/\Theta^{\ell}(E')}\left(\Theta^{\ell}(E')+E_j\right)}{\Theta^{\ell}(E')\left[\Theta^{\ell}(E')-e^{-E'/\Theta^{\ell}(E')}\left(\Theta^{\ell}(E')+E'\right)\right]}\Bigg] \Bigg/ \int_{E_{k+1}}^{E_k} dE'\ f(E')$$

where

$$\varepsilon'_{kj} = \begin{cases} 1 & \text{if} \quad E = \frac{M_{\ell}-1}{M_{\ell}+1}E' - \frac{M_{\ell}}{M_{\ell}+1}E_i \quad \text{and} \quad E \leq E' \leq E_k \quad \text{and} \quad E_{j+1} \leq E \leq E_j \\ 0 & \text{otherwise} \end{cases}$$

c/ The /n,2n/ process. For the energy distribution of neutrons arising from the /n,2n/ reaction the evaporation model is used, i.e. two neutrons are boiled off in succession with the mass number decreased by one for the second neutron.

$$2\Sigma^{k\to j}_{n,2n} =$$

$$= \sum_{\ell} Q_{\ell} \int_{E_{k+1}}^{E_k} dE'\ f(E')\,\sigma^{\ell}_{n,2n}(E') \sum_{s=1,2} \frac{e^{-E_{j+1}/\Theta^{\ell}_s(E')}\left(\Theta^{\ell}_s(E')+E_{j+1}\right)-e^{-E_j/\Theta^{\ell}_s(E')}\left(\Theta^{\ell}_s(E')+E_j\right)}{\Theta^{\ell}_s(E')\left[\Theta^{\ell}_s(E')-e^{-E'/\Theta^{\ell}_s(E')}\left(\Theta^{\ell}_s(E')+(E')\right)\right.}$$

where

$$\Theta^{\ell}_1(E) = \sqrt{\frac{E}{M_{\ell}}} \Big/ 0.31$$

$$\Theta^{\ell}_2(E) = \sqrt{\frac{E}{M_{\ell}-1}} \Big/ 0.31 \quad .$$

3. The evaluated data file available at IAEA

The evaluated data file available at IAEA is composed from KEDAK and AWRE files. At the present it contains 13 files. Their content and other parameters are given in Table 1. The detailed description of the KEDAK and

Table 1

File	For-mat	Numb.of char.in a block	Nuclei and types of data
1	AWRE	800	/n,γ/ cross-section for isotopes with mass number 83-160 /fission products/
2	KEDAK	800	For materials Al^{27}, C^{12}, Chromium, Iron, Deuterium, H^1 bound in H_2, H^1 bound in H_2O, He^4, Mo, Na^{23} - all types of data required for group constant calculation; for isotopes of Chromium, Iron and Molybdenum resonance parameters only; for He^3 absorption and /n,p/-cross-section only; for N^{14}-differential elastic scattering only.
3	KEDAK	800	For Ni, O^{16}, Pu^{239}, U^{235}-all types of data needed for group constant calculation; for isotopes of Ni-resonance parameters only.
4	KEDAK	800	For Cd, Pu^{240}, Pu^{241}, Pu^{242}, U^{235}-all types of data needed for group constant calculation.
5	AWRE	800	For Zr-all types of data needed for group constant calculation.
6	AWRE	800	For Th^{232}-all types of data needed for group constant calculation.
7	AWRE	800	For Be, Pu^{241}, B^{11}-all types of data needed for group constant calculation.
8	AWRE	800	Pu^{239}- all types of data needed for group constant calculation.
9	AWRE	800	For U^{235}- all types of data needed for group constant calculation.
10	AWRE	800	For U^{238}- all types of data needed for group constant calculation.
11	AWRE	800	/n,γ/ cross-section for isotopes with mass number 81-157 /fission products/.
12	AWRE	80	For Li^6- all types of data needed for group constant calculation.
13	AWRE	80	For Li^7- all types of data needed for group constant calculation.

AWRE format can be found in the reports [6] and [7], respectively. Here we restrict ourselves to the main features of these formats, discussing the essential differences between them.

a/ KEDAK format

At the beginning of each KEDAK file there is a description of material contents. At the beginning of data group for each material there is a description of data type contents.

The information is arranged in records of 80 characters /card-image format/. The 73-80 character positions are the identification part of the record.

73-74 are the positions at which the material appears in the description of the material contents,

75-76 are the positions at which the data type appears in the description of the data type contents,

77-80 are the serial number of the card in the given data group.

Before each data group there is a record containing the number of data sets in that group. If there are further parameters /e.g. energy of excitation level at inelastic scattering, or incident neutron energy for differential scattering cross-section, etc./, then they are given in a record before that containing the number of data sets. Each data group begins with the information on the material type, data type, number of further parameters, number of arguments and functional values, and number of different values of further parameters.

b/ AWRE format

One of the most essential and disconcerting differences between the KEDAK and AWRE format is in the identification of nuclei. In the AWRE files the data sets of a given material are identified with a number of three figures which is arbitrary chosen by the editors of the file. This number is placed in the 73-75 character positions of each record. The numbers placed in the 73-76 character positions of any KEDAK file are nondescending, and this is not true for AWRE files.

The identification of data groups for a given material is similar to that in KEDAK files, the only difference being that the 76-77 character positions serve for this purpose.

The energy range covered is divided into some particular intervals. Before the data group for each interval there can be found information on the

lower and upper limit of the interval, the material temperature, the number of data sets in this interval, and the number of temperatures still to be fully considered. Thus the number of data sets in the local energy range can not be recognized at once before the data group. This is also an uncomfortable feature of AWRE files.

There are differences not only in the form of the files but in their content too. Transport cross-sections are generally missing in the AWRE files. While in KEDAK files the differential elastic cross-sections are given, in AWRE files only the probability of angular distribution can be found /and, of course, the total scattering cross-section/. While in the KEDAK files the energy of excitation level is a further parameter, in the AWRE files the inelastic cross-sections for every excitation level are represented by separate data groups.

A great effort has been made in order to confine the effect of differences in data source on the structure of the program processing these data. This problem will be discussed in detail in the next section.

4. Stages of the production of multigroup constants

There are three stages in the calculation of multigroup constants from the evaluated data files. In any stage the calculation starts from a magnetic tape data file and the work is finished with a newly created magnetic tape data file. Each file has a specific and strictly defined structure characterizing the job performed in the stage. The evaluated file originating from IAEA will be denoted by DFO. The files created by the three stages are denoted by DF1, DF2, DF3, respectively.

While the file DFO is written by the special magnetic tape-handling subroutines for the ICL-1905 computer, the files DF1, DF2 and DF3 are written by the ICL standard FORTRAN system.

1st stage

The program searches the data groups of any given material and searches the data type for this material. The position of the data, i.e. characters 73-76 /for AWRE data 74-77/ of the data cards, should be specified by input paper tape. Data are read in, converted into binary form and written on to DF1 in a rearranged order.

For any material on the file DF1 there are at most 15 data types in a strictly definite order, as shown in Table 3. The structure and format of DF1 are given in Table 2.

Table 2.

Information type	List of I/O statement	Content
Introductory	KE/I/,NFU/I/,I=1,50	KE/I/,for I=-48, the name of materials contained in DF1; KE/49/, number of materials KE/50/, number of data types /15/ NFU/I/=n_i, where if n_i=0 or -2 then the i-th material is non-fissionable; if n_i = 1 the i-th material is fissionable; if n_i = 0 the i-th material is on an AWRE file, otherwise it is on a KEDAK file.
Records for a given material and data type,and, if there is a further parameter, then for a given value of it	KR/I/ I=1,6 *	KR(1)=K_1, number of data sets KR(2)=K_2, number of data records KR(3)=K_3, number of further parameters KR(4)=K_4, number of arguments KR(5)=K_5, number of functional values KR(6)=K_6, number of combinations of further parameters
	FN/I/, I=1,3	This record exists if K_3=0 FN(1)= the value of the further parameter; FN(2)= atomic mass of the material /only for AWRE data/
	NKR, AC/J/,DC/J/=1, NKR	NKR $\leq$ 2250 AC/J/argument, DC/J/functional value } repeated for each K_2
	IBS	Number of record for this data type
A record for a given material	IBN	Number of record for this material type

*If for a given data type the given material does not exist or is zero then K_1 = 0 and the records except the first and the last one are omitted.

Table 3.

No.	Name	Description and remarks
1	SGT3	total cross-section
2	STR3	transport cross-section in KEDAK, total cross-section in AWRE files
3	SGN3	elastic scattering cross-section
4	SGI3	total inelastic scattering cross-section
5	S2N3	cross-section for the /n,2n/ process
6	SGA3	absorption cross-section
7	SGG3	cross-section for /n,γ/ process
8	SAL3	cross-section for /n,α/ process
9	SGX3	nonelastic cross-section
10	SPR3	cross-section for /n,p/ process
11	SGE3	inelastic cross-section for excitation of rest nucleus level E_i
12	SNC4	differential elastic scattering cross-section in the center-of-mass system in KEDAK, and scattering probability in AWRE files
13	SGF3	fission cross-section
14	NUE3	average number of fission neutrons.
15	KHP3	energy spectrum of prompt fission neutrons

Remarks: 1/ except for SNC4, the argument is the neutron incident energy;

2/ E_i is a further parameter for SGE3;

3/ The neutron incident energy is a further parameter for SNC4.

It should be mentioned that because of the restricted fast memory capacity, there can be at most 2250 pairs of data in a record. The number of records for a given data type is indicated by K_2.

The differences between the KEDAK and AWRE data are much less on DF1 than on DFO. All differences vanish on DF2, i.e. at the end of second stage.

2nd stage

In this stage an energy argument system is introduced /EAS/ which is uniform for any materials and for any types of cross-section that are to be compiled together. The term "compiled together" will be clarified later. The total energy range in question /generally 0-10 MeV/ is divided into N intervals. This division will correspond to the multigroup system to be constructed. The intervals are divided into subintervals, i.e. a fine group system is introduced. The middle points of the fine group intervals constitute the above-mentioned EAS. The number of fine groups in a broad group may be quite large /$\leq$ 200/, thus allowing the fine structure of the cross-section to be followed.

The serial number of materials on DF1 to be compiled together on DF2 are specified by input. First the data of these material are scanned and copied on a scratch tapes while the record number of each data group is put down in a matrix. This matrix controls the data search on the type which has been copied from DF1.

The data are interpolated and written on the DF2 which is prepared in this stage. Above 1 eV the interpolation of data is performed linearly in lethargy, below 1 eV this is done linearly in energy.

The structure of DF2 is shown in Table 4. and it clarifies what we mean by the term "compilation". The DF2 file is organized so that the macroconstants of any mixture containing only the materials compiled together can easily be calculated in the next stage. Thus DF2 may be regarded as a generalized microgroup constant set which can be flexibly used for any purpose.

It should be mentioned that at the cost of some additional calculations all differences in KEDAK and AWRE data are eliminated.

3rd stage

In this stage macrogroup constants are produced by means of the formalism presented in the 2nd section. The calculated macroconstants are written on DF3. In a run we may calculate as many mixtures as we wish. The composition of the mixture is specified by input from tape.

The application of the formalism presented in Section 2 requires the determination of the flux and current and numerical integration over the group intervals. The flux and current are calculated by Eqs. /2.5/, and the numerical integrations are performed by a simple trapezoidal rule.

Table 4.

Information type	List of I/O statement	Content
Introductory	NDM,NG,NE,NF, /KFZ/I/,NFZ/I/,I=1,NE/ /M/I/, I=1,NG/, /UG/I/, I=1, NG+1/	NDM=the number of data type/15/ NG=number of broad group NE=number of materials NF=1 if the material is fissionable, NF=0 otherwise KFZ/I/ = KE/I/ NFZ/I/ = NFU/I/ M/I/=number of fine groups in the i-th broad group UG/I/=the upper boundary of the i-th broad group/in eV/

For the j-th data type j=1 - 10	k-th material	i-th broad group	ST/L/,L = 1,M/I/	values of the j-th data for k-th material, for the energy values EAS inside the i-th broad group

For the 11th data type	k-th material	i-th broad group	j-th energy values of EAS inside the i-th group	N,/E/L/, S/L/,L= 1,60/	N is the number of E/L/excitation energy values; S/L/is the corresponding inelastic cross-section
		i-th broad group	ST/L/,L=1,M/I/		total inelastic cross-section

12th data type	k-th material	i-th broad group	ST/L/,L=1,M/I/	elastic cross-section
		i-th broad group	j-th energy values of EAS inside the i-th group	ANU/L/,ASU/L/, L=1,21/	Angular values and values of corresponding differential elastic cross-section

k-th material	13th type	i-th broad group	ST/L/,L=1,M/I/	fission cross-section
	14th type	i-th broad group	ST/L/,L=1,M/I/	average number of neutron per fission

15th data type	k-th material	i-th broad group	ST/L/,L=1,M/L/	fission spectrum

Table 5.

Information type	List of I/O statements	Content
Introductory	NE,NG,NF,JLO,KE I AM I,RO I,I=1,NE	NE is the number of materials in the mixture; NG is the number of broad groups; NF=1 for fissionable mixture, NF=0 otherwise; JLO is the maximum group change in a collision; KE means the name of the materials, AM is its atomic mass, and RO is the nuclear density.
i-th group	/CRO/J/,CRT/J/,J=1,10/, /TRAN/J/,TRANI/J/,J=I,NG/, SF, SNF, HAS/I/	CRO/J/ and CRT/J/ are macro-cross-sections for data type j=1-10 averaged over the flux and current, respectively; TRAN/J/ and TRANI/J/ are transfer cross-sections, SF is the fission macro-cross-section; SNF is the average number of neutrons per fission; HAS/I/ is the fission spectrum.

5. Description of the functions and subroutines of the program

Corresponding to the three stages discussed in the previous section, there are three main subroutines: DATFIL, CONSTP1 and GROUP. Another three subroutines CONTROL, OUTLIST, EDITOR respectively check the results of their work

D A T F I L

DF0 and DF1 are opened in DATFIL, and the job concerning the first stage is performed by means of the following related subroutines:

ARED- reads the next record of 80 characters on DF0 and places them in an array which serves as an input periphery

FINDELEM- searches the first record of a given material on DF0

FINDKEDAK - searches the first record of a given data type for the material in question /data must be in KEDAK format/

FINDAWRE - does the same job as FINDKEDAK but for data in AWRE format

DARE - converts and rearranges the data which are in KEDAK format and edits the DF1

AWDARE - does the same job as DARE but for data in AWRE format

CONTROL

This procedure performs a checking output for a given material and given data type on DF1.

C O N S T P 1

DF2 is opened in CONSTP1 and the job concerning the second stage is performed by means of the following related subroutines and functions:

HELYMEG - puts down the place number of data records to be searched on the scratch tape prepared by copying DF1

TOLTELEM - copies the data from DF1 on to a scratch tape

FORELEM - scans the data groups on DF1

SIG /function/ - calculates the cross-section on the energy points of EAS by averaging over the fine group interval

BSIG /function/ - supplies any cross-section value at a given energy point by interpolating data values on DF1

SEARCH - searches a given data type for a given material on DF1

CINT /function/ - performs the interpolation in energy

ΘLV - reads the arguments and cross-section values from DF1

ESIG - supplies the inelastic cross-section at a given energy point for all excitation level lower than this energy

SITRAN - calculates the transport cross-section in the case of AWRE data

NUSIG - supplies the differential elastic scattering cross-section at a given energy.

O U T L I S T

This subroutine performs a checking output for a given data type of all materials on DF2.

G R O U P

DF3 is opened in GROUP and the job concerning the third stage is performed by means of the following related functions and subroutines:

MIXOLV - reads in the cross-section data for a given group for all materials and produces the macro cross-sections for all energy points inside the group

FLUXUS - calculates f(E) and j(E) for all energy points inside the group, making use of $\Sigma_{tot}(E)$ and $\Sigma_{tr}(E)$ calculated by MIXOLV

SINT - performs the numerical integration by trapezoidal rule

IRG /function/ -supplies the serial number of that group to which a given energy value belongs

ASPN /function/ - interpolates the differential scattering cross-section by angular variable

DIV - calculates the energy distribution by the evaporation model.

E D I T O R

This subroutine performs a checking output of all macrogroup constants for a given group.

The connections between the subroutines and functions are shown in the block diagram /Fig. 1./. Roman numbers indicate the overlay structure of the program; i.e. subroutines with the same Roman number are in the same layer.

6. Versions for program operations and the description of the input

By use of a switch number any of the stages can be operated separately if the corresponding input DF is available /e.g. it has been prepared in an earlier run/. Thus, for instance, if we have a library of type DF2 for a given set of materials, the group constants of any mixture consisting of some of these materials can be calculated immediately by operating the third stage only.

The input paper tape is described by stages. The input format is a free one, that is the items are separated by two spaces; only the number of items in a line is restricted.

Input for the 1st stage

LINE	FORMAT	VARIABLES	DESCRIPTION
1	IO	KN	Number of materials on DF1 to be prepared

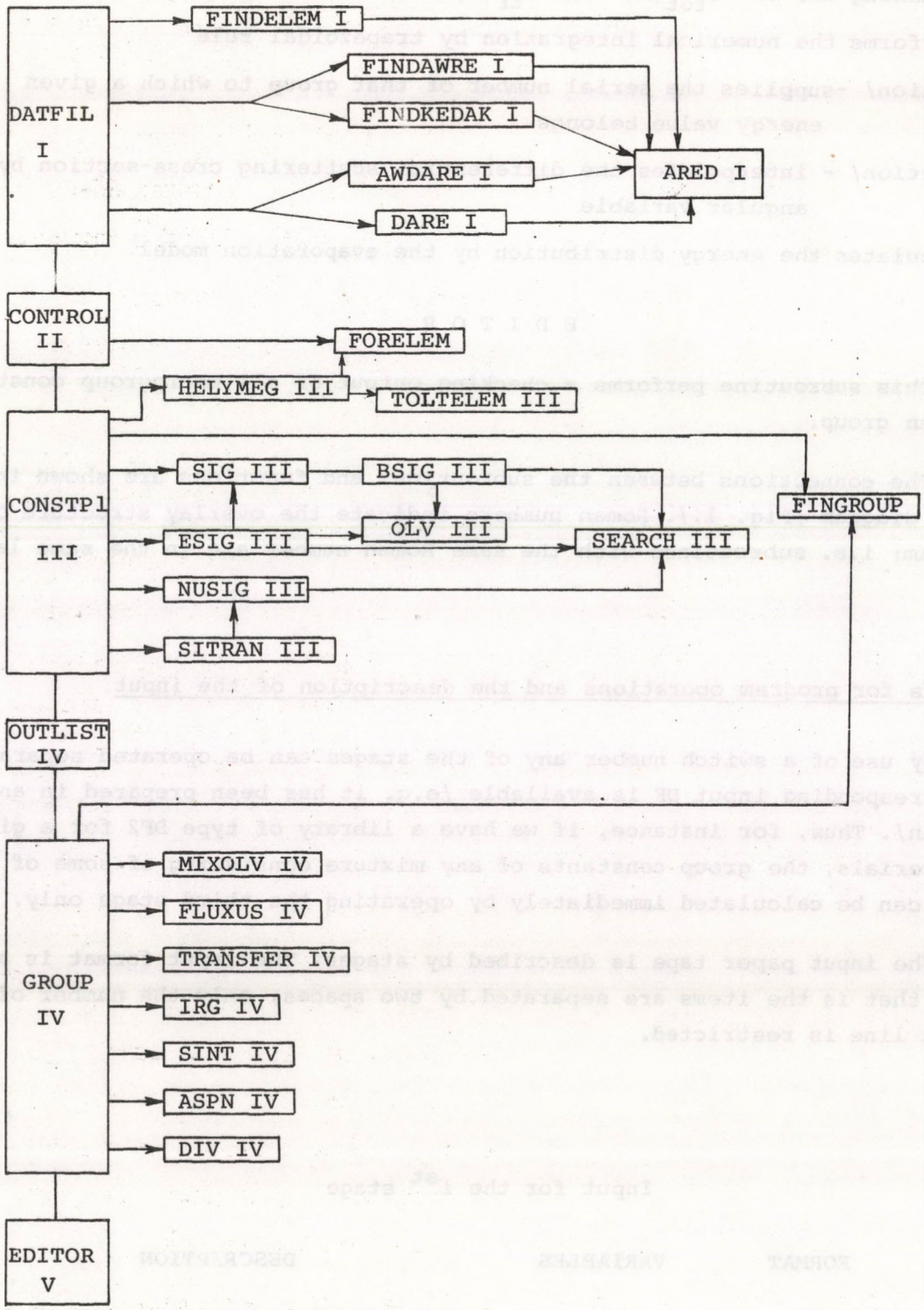
DATFIL I
FINDELEM I
FINDAWRE I
FINDKEDAK I
AWDARE I
DARE I
ARED I
CONTROL II
FORELEM
HELYMEG III
TOLTELEM III
CONSTPl III
SIG III
BSIG III
OLV III
ESIG III
SEARCH III
NUSIG III
SITRAN III
FINGROUP
OUTLIST IV
GROUP IV
MIXOLV IV
FLUXUS IV
TRANSFER IV
IRG IV
SINT IV
ASPN IV
DIV IV
EDITOR V

Fig. 1

LINE	FORMAT	VARIABLES	DESCRIPTION
2	A4,2X,A8,IO	KE(I),SNE*(I), NFU(I)	KE(I) is the name of the material /in four characters/. SNE(I) : the last two characters give the name of the subfile in which the given material can be found on DFO; the 3rd character is 2 for KEDAK files, 3 for AWRE ones; 4th and 5th characters are arbitrary; characters 6-7 or 6-8 are the identification number of material. NFU(I) is n_i /see Table 2./
3	5(A4,2X)	NK*(J)	Data type identification numbers

Only for AWRE data:

LINE	FORMAT	VARIABLES	DESCRIPTION
4	IO,1O 2X,A4	KR(6),NK(I+2O), I=1,KR(6)	KF(6) is the number of inelastic scattering levels. NK(I+2O) are the identifications of data for these levels.

Remarks: 1/ Lines 3 and 4 are repeated for each material.

2/ If a data type for a material does not exist or is zero, then the last two characters of NK(J) should be 00.

Input for CONTROL

1	17IO	IE,JX,JD(I),I=1,JX	IE = the serial number of material on DF1 to be checked: JX is the number of data types; JD(I) is the serial number of data to be printed out.

Remarks: 1/ IE and JX should be given in a strictly increasing order

2/ If IE=0 then the work of CONTROL is terminated.

---

* Characters for SNE and NK can be found in Table 6.

Input for 2nd stage

LINE	FORMAT	VARIABLES	DESCRIPTION
1	2IO,FO.O	NG,NU,T	NG is the number of broad group : if NU=O, then the broad group boundaries are the same as for the Abagyan set [2]; if NU=O, then they should be specified by input. T is the temperature
2	1OIO	M/I/,I=1,NG	Number of fine groups in the broad groups
3	1OFO.O	UG/I/,I=1,NG	Broad group boundaries /this line is present unless NU=O/
4	3IO	NIS,NF,NE	NIS=O if there are not more groups of materials to be compiled together, NIS=O otherwise; if there are fissionable materials among those to be compiled then NF=O, otherwise NF=O; NE is the number of materials.
5	1OIO	NTM/I/,I=1,NE	The serial number of material on DF1

Input of OUTLIST

1	1OIO	JD,NX,JGX/I/,I=1,NX	JD is the data type number; NK is the number of broad groups for which fine group cross-section of JD data type are to be printed out. JGX(I)are the broad group indices

Remarks: 1/ JD and JGX should be given in a strictly increasing order,

2/ if NX=O but JD=O, then the next compilation is taken;
if NX=JD=O, then the job of OUTLIST is terminated.

Input for the 3rd stage

1	FO.O,2IO	T,NF,NE1,JLO	T is temperature; NF has the same meaning as in the 2nd stage; NE1 the number of material in the mixture; JLO is the maximum group change by a scattering /at present this is $\leq$ 1O/

LINE	FORMAT	VARIABLES	DESCRIPTION
2	A4,2FO.O	KFZ(I),AMZ(I),RZ(I), I=1,NE1	KFZ = material name AMZ = atomic mass RZ = nuclear density
3	IO	J	J=O if no further mixture to be calculated, J=O otherwise.
		Input for EDITOR	
1	IO	IG	IG is the broad group index for which the transfer cross-section should be printed if IG=O, EDITOR is terminated if IG=O, the cross-sections are punched out.

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Table 6/a.

Material name	Format	SNE	SGT3	STR3	SGN3	SGI3	S2N3	SGA3	SGG3	SAL3	SGX3	SPR3	SGE3	SNC4	SGF3	NUE4	KMP3
H-1B	KEDAK	EG24 14	14 8	14 9	14 6	14 5	1411	14 2	14 4	14 3	141o	14 7	14oo	14oo	14oo	14oo	14oo
H2OB	KEDAK	EG24 15	15 8	15 9	15 6	15 5	1511	15 2	15 4	15 3	151o	15 7	15oo	15oo	15oo	15oo	15oo
DE-2	KEDAK	EG24 13	1311	1312	13 8	13 7	1314	13 4	13 6	13 5	1313	131o	13oo	13 9	13oo	13oo	13oo
HE-4	KEDAK	EG24 17	1711	1712	17 8	17 7	1714	17 4	17 6	17 5	1713	171o	17oo	17 9	17oo	17oo	17oo
LI-6	AWRE	1133 214	oo 1	oo 1	oo 2	oooo	oo1o	oooo	oo13	oo15	oo 4	oo14	oo 5	oo 3	oooo	oooo	oooo
LI-7	AWRE	1233 215	oo 1	oo 1	oo 2	oo13	oo 7	oooo	oo16	oo17	oo 4	oooo	oo 5	oo 3	oooo	oooo	oooo
BE-3	AWRE	EN33 5o	oo 1	oo 1	oo 2	oooo	oo 5	oooo	oo 8	oo1o	oo 4	oo 9	oooo	oo 3	oooo	oooo	oooo
B-11*	AWRE	EN33 49	oo 1	oo 1	oo 2	oo1o	oooo	oooo	oo13	oo16	oooo	oo14	oo 4	oooo	oooo	oooo	oooo
C-12	KEDAK	EG24 2	213	214	21o	2 8	216	2 5	2 7	2 6	215	212	2 9	211	2oo	2oo	2oo
O-16	KEDAK	EH24 7	713	714	71o	7 8	716	7 5	7 7	7 6	715	712	7 9	711	7oo	7oo	7oo
NA23	KEDAK	EG24 27	2713	2714	271o	27 8	2716	27 5	27 7	27 6	2715	2712	27 9	2711	27oo	27oo	27oo
AL27	KEDAK	EG24 1	113	114	11o	1 8	116	1 5	1 7	1 6	115	112	1 9	111	1oo	1oo	1oo
CROM	KEDAK	EG24 3	314	315	311	3 9	317	3 6	3 8	3 7	316	313	31o	312	3oo	3oo	3oo
FEOO	KEDAK	EG24 8	814	815	811	8 9	817	8 6	8 8	8 7	816	813	81o	812	8oo	8oo	8oo
NIOO	KEDAK	EH24 1	114	115	111	1 9	117	1 6	1 8	1 7	116	113	11o	112	1oo	1oo	1oo
ZR91	AWRE	EK33 9	oo 1	oo 1	oo 2	oo 5	oo 8	oo11	oooo	oooo	oo 4	oooo	oooo	oo 3	oooo	oooo	oooo
CDOO	KEDAK	EI24 1	111	112	o 9	1 7	114	1 4	1 6	1oo	113	11o	1 8	1oo	1oo	1oo	1oo
MOOO	KEDAK	EG24 18	1814	1815	1811	18 9	1817	18 6	18 8	18 7	1816	1813	181o	1812	18oo	18oo	18oo
TH32	AWRE	EM33 22	oo 1	oo 1	oo 2	oo 5	oo 8	oooo	oo18	oooo	oo 4	oooo	oooo	oo 3	oooo	oooo	oooo
U235	KEDAK	EH24 9	92o	921	917	915	923	911	914	912	922	919	916	918	913	9 8	9 3
U235*	AWRE	EQ33 o66	oo 1	oo 1	oo 2	oo23	oo26	oooo	oo36	oooo	oo 4	oooo	oo 5	oo 3	oo32	oo35	oo34
U238	KEDAK	EI24 5	518	519	515	513	521	5 9	512	51o	52o	517	514	516	511	5 6	5 2
U238*	AWRE	ER33 4o1	oo 1	oo 1	oo 2	oo35	oo38	oooo	oo48	oooo	oo 4	oooo	oo 5	oo 3	oo44	oo47	oo46
PU39	KEDAK	EH24 8	82o	821	817	815	823	811	814	812	822	819	816	818	813	8 8	8 3
PU39*	AWRE	EP33 o65	oo 1	oo 1	oo 2	oo19	oo22	oooo	oo32	oooo	oo 4	oooo	oo 5	oo 3	oo28	oo31	oo3o
PU4	KEDAK	EI24	217	218	215	213	216	21o	212	2oo	219	2oo	214	216	211	2 7	2oo
PU41	KEDAK	EI24 3	317	318	315	313	316	31o	312	3oo	319	3oo	314	316	311	3 7	3oo
PU41	AWRE	EN33 6o	oo 1	oo 1	oo 2	oo 5	oo 8	oooo	oo18	oooo	oo 4	oooo	oooo	oo 3	oo14	oo17	oo16
PU42	KEDAK	EI24 4	417	418	415	413	416	41o	412	4oo	419	4oo	414	416	411	4 7	4oo

* = Inelastic scattering for distance excitation levels for AWRE data.

Table 6/b.

Material name	Number of levels	2	3	4	5	6	7	8	8	lo
B-11	3	oo 6	oo 8							
U235	6	oo 8	ooll	ool4	ool7	oo2o				
U238	lo	oo 8	ooll	ool4	ool7	oo2o	oo23	oo26	oo29	oo32
PU	7	oo 7	oo 9	ooll	ool3	ool5	ool7			

61.869

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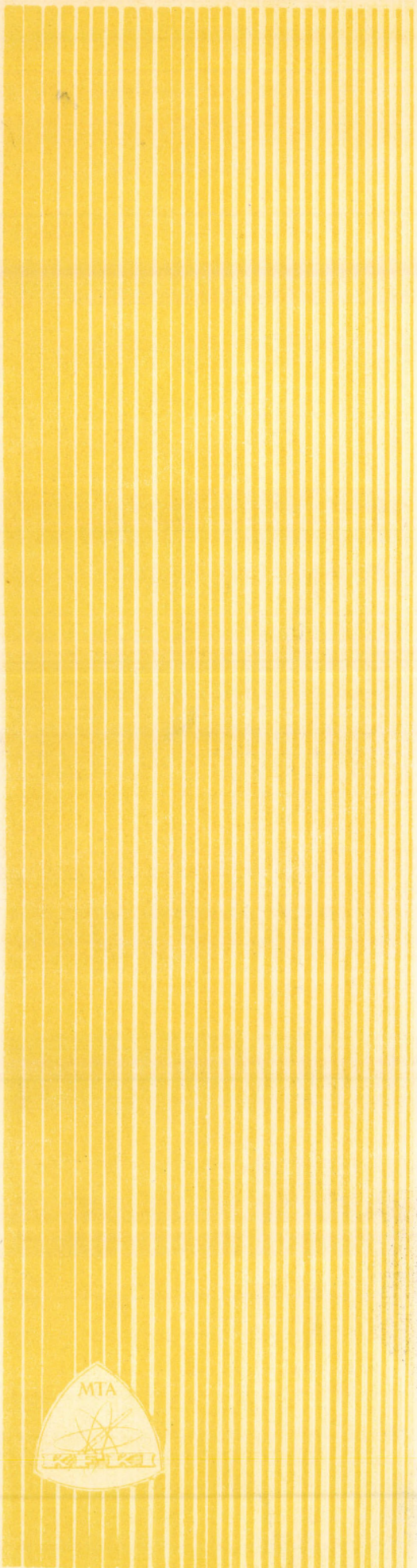

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